JS 6/2/21
RJA 2/18/22

Ecotox Report for Case # P-19-0025

General

[redacted]

Report Status: Complete
Status Date: 12/28/2018
CRSS Date: 11/29/2018
SAT Date: 11/30/2018
SAT Chair: Rebecca Daiss
Consolidated PMN: N
Consolidated Set:
Ecotox Related Cases: [redacted]
Health Related Cases:
Submitter: Bercen, Inc.
CAS Number: 62978-77-2
Chemical Name: 11-Docosene
Use: [redacted] Analogues (same use): None. Patents (same use): None.
Trade Name: None
PV-max(kg/yr): [redacted]
Ecotox Assessor: Wright, Tracy

Fate Summary Statement

Fate Summary Statement:

P-19-0025
FATE:

Liquid with MP < 20 °C (M)
log Kow = 10.9 (E)
S < 0.001
mg/L at 25 °C (E)
VP = 1.5E-4 torr at 25 °C (E)
BP = 361 °C (E)
H
= 3.94E+1 (E)
log Koc = 6.29 (E)
log Fish BCF = 1.60 (40)
(E)
log Fish BAF = 3.94 (8,600) (E)
POTW removal (%) = 90-95 via

sorption and biodeg
Time for complete ultimate aerobic biodeg =
wk
Sorption to soils/sediments = v.strong
Volatilization half-life
from a standard river = 2 hrs
Volatilization half-life from a standard
lake = 7 da
Atmospheric Oxidation Half-life = 1.6 hr via OH
radical
Atmospheric Oxidation Half-life = 2.1 hr via ozone
PBT
Potential: PB1
FATE: Migration to ground water =
negl
Bioconcentration factor to be put into E-FAST:
40

Physical Chemical Information

Molecular Weight: 308.6

Wt% < 500: **Wt% < 1000:**

Physical State - Neat: Liquid

Melting Point: **Melting Point (est):** <20

MP (EPI): NaN °C
(Exp.) 59.46002197265625 °C (Est., Joback) 97.242431640625 °C (Est., Gold)
68.90562438964844 °C (Est., Selected)

Vapor Pressure: **Vapor Pressure (est):** 0.00015

VP (EPI): NaN mmHg
(Exp.) 0.003308588770483766 Pa (Est., Antoine) 2.4816525183268823E-5 mmHg
(Est., Antoine) 0.007898312559155036 Pa (Est., Grain) 5.924237979594542E-5
mmHg (Est., Grain) 0.00701656487744471 Pa (Est., Mackay) 5.262871002118713E-5 mmHg (Est., Mackay) 0.007898312559155036 Pa (Est.,
Selected) 5.924237979594542E-5 mmHg (Est., Selected) 0.020441590274887858
Pa (Est., SubCooled) 1.5332495968323 2E-4 mmHg (Est., SubCooled)

Water Solubility (est): <0.000001

Water Solubility:	
Water Solubility (EPI):	NaN (Exp.) 1.4691919432152645E-6 (Est.)
Henry's Law::	NaN atm-m3/mole (Exp.) 39.39784622192383 atm-m3/mole (Est., Bond) 111.8037338256836 atm-m3/mole (Est., Group)
Log Koc:	NaN
Log Koc (EPI):	14.481831678314546 (Est., log(MCI)) 16.88239238901847 (Est., log(Kow)) 1947061.125 L/kg (Est., MCI) 2.1474836E7 L/kg (Est., Kow)
Log Kow:	
Log Kow (EPI):	NaN (Exp.) 10.93 (Est.)
Log Kow Comment:	

SAT Concern Level

Ecotox Rating (1):	1
Ecotox Rating Comment (1):	
Ecotox Rating (2):	
Ecotox Rating Comment (2):	
Ecotox Route of Exposure:	No releases to water

Ecotox Comments

Exposure Based Review (Eco):	Y
Ecotox Comments:	
Exposure Based Testing:	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments
2	1		

Eco-Toxicity Comment:

Fate Ratings

Removal in WWT/POTW (Overall):	90-95					
Condition	**Rating Values**	**Rating Description**				**Comment**
		1	**2**	**3**	**4**	
Fish BCF:	3.16 L/kg wet-wt					
Log Fish BCF:	NaN (Exp.) 0.5 (Est.)					
WWT/POTW Sorption:	3	Low	Moderate	Strong	V. Strong	
WWT/POTW Stripping:	4	Extensive	Moderate	Low	Negligible	
Biodegradation Removal:	2	Unknown	High	Moderate	Negligible	
Biodegradation Destruction:	2-3	Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	2	<= Days	Weeks	Months	> Months	
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	3	<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Hydrolysis (t1/2 at pH 7,25C) A:		<= Minutes	Hours	Days	>= Months	
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:	1	V. Strong	Strong	Moderate	Low	
Migration to Ground Water:	1	Negligible	Slow	Moderate	Rapid	
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	

Removal in WWT/POTW (Overall):	90-95					
Condition	**Rating Values**	**Rating Description**				**Comment**
		1	**2**	**3**	**4**	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	
Bio Comments:	Fish log BAF = 3.94 (8,600). The fugacity spreadsheet and the EPI output file for thPMN material is attached.					
Fate Comments:						

Ecotoxicity Values

Test organism	**Test Type**	**Test Endpoint**	**Predicted**	**Experimental**	**Comments**
Fish	96-h	LC50	*		* = no effects at saturation (Neutral Organics QSARs)
Daphnid	48-h	LC50	*		"
Green Algae	96-h	EC50	*		"
Fish	-	Chronic Value	*		"
Daphnid	-	Chronic Value	*		"
Green Algae	-	Chronic Value	*		"

Ecotox Value Comments: Predictions are based on QSARs for neutral organics (ECOSAR V2.0); MW 309; Log Kow = 10.93 (P); liquid with an unknown MP (P);
S = 1.9E-06 (P); effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150 mg/L as CaCO3; and TOC <2.0 mg/L

Ecotox Factors

Factors	**Most Sensitive Endpoint**	**Assessment Factor**	**CoC**	**Comment**
Acute Aquatic (ppb):	NES			Because hazards are not expected up to the water solubility limit, acute and chronic

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
				concentrations of concern are not identified.
Chronic Aquatic (ppb):	NES			Because hazards are not expected up to the water solubility limit, acute and chronic concentrations of concern are not identified.

Factors	Values	Comments
SARs:	Neutral Organics	
SAR Class:	Neutral organics-hydrocarbon	
TSCA NCC Category?	Neutral Organics	

Recommended Testing: Potentially Useful Information: None

Ecotox Factors Comments: Environmental Hazard: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risk because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using the Ecological Structure Activity Relationships (ECOSAR) Predictive Model (https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model; specifically the QSAR for neutral organics. Acute toxicity values estimated for fish, aquatic invertebrates, and algae are all no effects at saturation. Chronic toxicity values estimated for fish, aquatic invertebrates, and algae are all no effects at saturation. These toxicity values indicate that the new chemical substance is expected to have low environmental hazard. Because hazards are not expected up to the water solubility limit, acute and chronic concentrations of concern are not identified.

Environmental Risks: Risks to the environment were evaluated by comparing estimated surface water concentrations with the acute and chronic concentrations of concern. Risks to the environment from acute and chronic exposure are not expected at any concentration of the new chemical substance soluble in the water (i.e., no effects at saturation)

Comments/Telephone Log

Artifact	Update/Upload Time